IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater–Revised and Updated Part 1. C_5 Hydrocarbons with Water

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The mutual solubility and related liquid–liquid equilibria of C_5 hydrocarbons with water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 13 chemically distinct binary systems for which data appeared in the primary literature prior to end of 2002 are compiled. For seven systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of the all experimental data for a given homologous series of saturated or unsaturated aliphatic hydrocarbons was used. © *2005 American Institute of Physics.*
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Key words: C_5 hydrocarbons; critical evaluation; liquid–liquid equilibria; solubilities; water.

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1. Preface

1.1. Scope of This Volume

The solubilities of binary systems of C_5-C_{36} hydrocarbons with water, heavy water, and seawater were reviewed in 1989 in Volumes 37 and 38 of the IUPAC Solubility Series.[1,2] Because solubilities of hydrocarbon-water systems are of considerable importance and widespread interest among several groups including industrial and environmental chemists, because the earlier volumes are now difficult to obtain and nearly 20 years out of date (for most systems, compilation ended in the mid-1980s), and because a new technique of data evaluation has been developed, the decision was made to revise and update this work as a new volume. This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) and contains new compilations based on recent and previously overlooked reports, and new evaluations for systems where two or more independent measurements of solubility have been reported.

The revised work is volume 81 in the Solubility Data Series and will be published in 12 parts as listed below.

Part 1: C_5 Hydrocarbons with Water (13 systems; 7 evaluations)

Part 2: Benzene with Water and Heavy Water (2 systems; 1 evaluation)

Part 3: C_6H_8-C_6H_{12} Hydrocarbons with Water and Heavy Water (12 systems; 6 evaluations)

Part 4: C_6H_{14} Hydrocarbons with Water (5 systems; 5 evaluations)

Part 5: C_7 Hydrocarbons with Water and Heavy Water (22 systems; 9 evaluations)

Part 6: C_8H_8-C_8H_{10} Hydrocarbons with Water (5 systems; 5 evaluations)

Part 7: C_8H_{12}-C_8H_{18} Hydrocarbons with Water (20 systems; 5 evaluations)

Part 8: C_9 Hydrocarbons with Water (18 systems; 8 evaluations)

Part 9: C_{10} Hydrocarbons with Water (19 systems; 10 evaluations)

Part 10: C_{11} and C_{12} Hydrocarbons with Water and Heavy

Water (22 systems; 11 evaluations)
Part 11: C_{13}-C_{36} Hydrocarbons with Water (46 systems; 18 evaluations)
Part 12: C_5-C_{26} Hydrocarbons with Seawater (46 systems, 15 evaluations)

To the extent allowed by the available data, this volume treats mutual solubility. That is, data for both the solubility of a hydrocarbon in water and water in that hydrocarbon are compiled and evaluated together, when available. For a few systems in Parts 2, 3, 5, and 10, mutual solubility data with heavy water (D_2O) are also included. Solubilities of hydrocarbons in seawater are grouped together in Part 12. A variety of units for the expression of solubility have appeared in the primary literature. For the purpose of comparison the compilers of this volume have, so far as possible, expressed all original results in terms of mass percent and mole fraction as well as the units reported by the original investigators. Where conversions have been made, these are attributed to the compiler and the source of any auxiliary data not provided by the original investigators (such as hydrocarbon or seawater density) is specified. Definitions of mass percent and mass fraction as well as their relationship to other commonly used measures of solubility are given in the Introduction to this volume.

Experimental methods for determining hydrocarbon water solubility can be categorized as either synthetic or analytical. One widely used synthetic method is the cloud point technique, in which one component is titrated with the other until turbidity or its absence is observed, depending on the direction from which equilibrium is approached. With careful temperature control and adequate stirring, it is possible to cross back and forth over the end point several times and obtain precise results by averaging. The method is only applicable if both components are liquids at the temperature of the experiment. In a modification of the synthetic method precisely measured amounts of the two components are sealed into a glass ampoule, which is then heated or cooled as necessary to determine temperature of solubility by observation of the cloud point. In this variation the system pressure at which solubility is observed is unknown. However, since the effect of pressure on solubility is generally small, it is often ignored.

In the analytical method a saturated solution, either of hydrocarbon in water or water in hydrocarbon, is prepared and its composition is determined. When water is the continuous phase hydrocarbons are determined by a variety of techniques with gas chromatography and optical spectrometry being common. When the hydrocarbon is the continuous phase water is almost always determined by the Karl Fischer method. The success of the analytical technique is critically dependent on the preparation of a saturated solution, which can be difficult especially for high molecular weight hydrocarbons whose water solubility is very low. The presence of only a small amount of the minor component adsorbed to surfaces or in the form of colloidal droplets can significantly influence the results obtained. This can lead to major positive systematic errors. For the best hydrocarbon in water measurements it is necessary to ensure that the water used is free of dust and other particles since sorption of hydrocarbons to surfaces can be significant. One measure of the presence or absence of small particles is the Tyndall Effect. If a saturated solution is prepared by shaking the components together, it is important to ensure that particles are not formed and again the Tyndall Effect is useful. Unfortunately, lack of experimental detail in some published reports makes error evaluation difficult. As an alternative to shaking or stirring components to achieve equilibrium, some workers have used a ''generator column'' in which water is passed through a bed of glass beads or other inert support which were previously coated with the hydrocarbon component. To establish that saturation has been reached, the generator column pathlength is increased until the concentration of hydrocarbon remains constant. Users of this volume are advised to be aware of potential sources of error in these measurements, especially for systems where only one or a few measurements have been made or when solubilities are very low.

This volume is the result of a careful search of the chemical literature. The goal of that search was to include all published data for the systems indicated in the title. Each evaluation includes a closing date for the literature search of that system, usually January 2003 or later. In spite of these efforts, some published measurements may have been missed. The editors will appreciate having their attention brought to any overlooked source of solubility data.

1.2. Procedures Used in Critical Evaluation

When each system is evaluated separately the estimation of data quality can be difficult. For example, plots of solubility against temperature from two studies of the same system can yield two smooth but disagreeing curves, for which the source of the systematic difference is unclear. In other systems, only few experimental points are available. Moreover, solubilities in hydrocarbon water systems are very low and consequently even small experimental errors may lead to substantial relative errors in measured solubilities, which in some cases reach 100% or more. To help clarify these uncertainties this work presents a new approach to the critical evaluation of the solubility data of the hydrocarbon-water systems by the calculation of ''reference data'' using smoothing equations that incorporate solubility information from many systems. The calculation of reference data consists of two steps:

(1) Approximation of solubilities of hydrocarbons in water with a smoothing equation described in the next section. This equation depends on the hydrocarbon properties but contains also empirical coefficients. The same values of these coefficients are used for mixtures of *n*-alkanes, branched alkanes, cycloalkanes, and unsaturated hydrocarbons in water. They are derived from simultaneous regression of the hydrocarbon solubility data.
(2) Liquid-Liquid Equilibrium (LLE) calculations yielding solubility of water in various hydrocarbons. The input data for these calculations are the hydrocarbon in water

solubilities predicted with the smoothing equation. The LLE calculations use an equation of state (ESoC) modified to account for the role of hydrogen bonding in solvation.[4–6]

In these two steps an extensive body of experimental data is described with a few adjustable parameters providing an additional framework for comparison of experimental data and help in the recognition of systematic error. The hydrocarbon solubilities calculated from the smoothing equation and the calculated water solubilities are used as the reference data in evaluations. Maczynski and co-workers[3–5] have described the calculations and examples of the evaluation of data.

Derivation of Reference Data for Solubility of Hydrocarbons in Water

The mole fraction of hydrocarbon in water (x_1) along the three-phase equilibrium line is related to the heat of solution of the hydrocarbon ($\Delta_{\text{sln}}h$).

$$\partial \ln x_1 / \partial(1/T) = -\Delta_{\text{sln}}h/\text{R}. \tag{1}$$

Minimum solubility ($x_{1,\text{min}}$) occurs when $\Delta_{\text{sln}}h = 0$, which is generally observed near room temperature (T_{min}). Thus, linear dependency of $\Delta_{\text{sln}}h$ on temperature can be expressed as follows:

$$\Delta_{\text{sln}}h/\text{R} = (\Delta_{\text{sln}}C_p/\text{R})(T - T_{\text{min}}), \tag{2}$$

where $\Delta_{\text{sln}}C_p$ is heat capacity of the solution. Introducing this expression into Eq. (1) upon integration gives Eq. (3).

$$\ln x_1 = \ln x_{1,\text{min}} + (\Delta_{\text{sln}}C_p/\text{R})[T_{\text{min}}/T + \ln(T/T_{\text{min}}) - 1]. \tag{3}$$

Solubility of a hydrocarbon depends on the size of the cavity in the water needed to accommodate the dissolved molecule. This size is proportional to the excluded volume (b) of the hydrocarbon. Here the *Redlich-Kwong* Equation of State (RK EoS) is used and b is calculated from critical temperature (T_c) and critical pressure (P_c) with Eq. (4):

$$b = 0.08664 \cdot RT_c/P_c. \tag{4}$$

It was found (see Maczynski and co-workers[4,5]) that both $\ln x_{1,\text{min}}$ and $(\Delta_{\text{sln}}C_p/R)$ depend linearly on b. The relation for $\ln x_{1,\text{min}}$ was obtained from experimental points shown in Figs. 1 and 2. They were selected from available hydrocarbon solubility data measured in the vicinity of the minimum where $\ln x_1 \approx \ln x_{1,\text{min}}$. An abundance of data allows estimation of $x_{1,\text{min}}$ more accurately than solubilities at other temperatures. As shown by the figures the solubility at minimum can be approximated with Eq. (5):

$$\ln x_{1,\text{min}} = c_1 + c_2 b + c_\pi \cdot L, \tag{5}$$

where L is number of π-bonds in the molecule, e.g., $L=1$ for alkenes, $L=2$ for alkadienes and alkynes, and $L=4$ for alkadiynes. When $L=0$, Eq. (5) describes minimum solubility of *n*-alkanes, branched alkanes, and cycloalkanes shown in Fig. 1. The line in Fig. 1 was adjusted to the points yielding values of c_1 and c_2. Using these values the coefficient

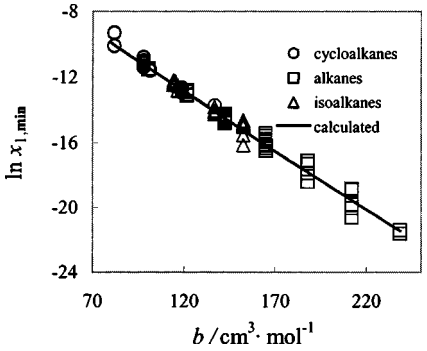

FIG. 1. Minimum solubilities ($x_{1,\text{min}}$) of alkanes in water vs excluded volume (b).

c_π was fitted to the points shown in Fig. 2. The following values were obtained: $c = -4.08'c_2 = -/0.073$ mol·cm^{-3}, $c_\pi = 1.10$ or $c_\pi = 0.79$ (for conjugated π-bonds).

The standard error of Eq. (5) is obtained from the variance-covariance matrix in the least squares method is as follows:

$$s(\ln x_{1,\text{min}}) = (D_{11} + 2 \cdot D_{12} \cdot b + D_{22} \cdot b^2 + D_{33} \cdot L_\pi^2)^{0.5}, \tag{6}$$

where $D_{11} = 0.010$; $D_{12} = -7 \cdot 10^{-5}$ mol·cm^{-3}; $D_{22} = 5 \cdot 10^{-7}$ mol^{-2}·cm^{-6}; $D_{33} = 0.0011$.

Equation (5) is useful for identification of outlying experimental data not only at the minimum but also at other temperatures, because the corresponding experimental points should lie on a curve going through $\ln x_{1,\text{min}}$ predicted with Eq. (5). Therefore, this equation is a point of departure for the next stages of the evaluation. For hydrocarbons investigated here the coefficient $\Delta_{\text{sln}}C_p/R$ in Eq. (3) is proportional to b:

$$\Delta_{\text{sln}}C_p/R = c_3 \cdot b. \tag{7}$$

The value of c_3 was obtained by regression of the solubility data for alkanes with Eq. (3) where $T_{\text{min}} = 298$ K for cyclic

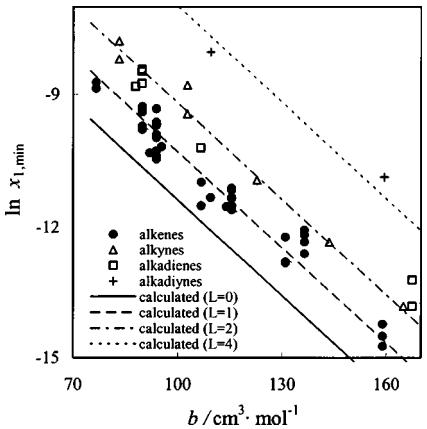

FIG. 2. Minimum solubilities ($x_{1,\text{min}}$) of unsaturated hydrocarbons in water vs excluded volume (b).

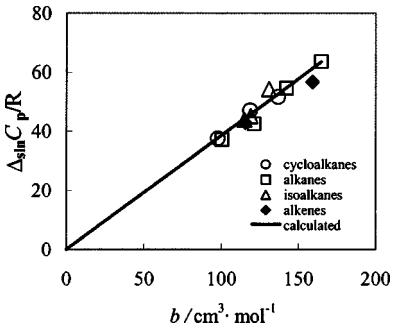

FIG. 3. Heat capacities of solution of the hydrocarbons ($\Delta_{sln}C_p$) vs excluded volume of hydrocarbon (b).

hydrocarbons and at $T_{min}=306$ K for other mixtures. During this regression $\ln x_{1,min}$ was fixed by Eq. (5). Values of c_3 and its standard error, $s(c_3)$ are as follows:

$$c_3 = 0.376 \text{ cm}^{-3}\cdot\text{mol}, \tag{8a}$$

$$s(c_3) = 2.6\cdot 10^{-3} \text{ mol}\cdot\text{cm}^{-3}. \tag{8b}$$

Maczynski *et al.*[4] and Góral.[5] have provided details of these calculations. The validity of Eq. (7) is illustrated in Fig. 3.

The hydrocarbon solubilities calculated from these equations are called here "reference data." It should be noted, however, that Eqs. (5) and (7) may not be appropriate outside the range of experimental data that were used for establishing of these equations. Their accuracy can be estimated with Eqs. (6) and (8b). For example, if one assumes $L=0$, then at $T=T_{min}$ from Eq. (6), one obtains the standard error $s(\ln x_{1,min})=0.032$ for $b=100\text{ cm}^3\cdot\text{mol}^{-1}$ and $s(\ln x_{1,min})=0.045$ for $b=200\text{ cm}^3\cdot\text{mol}^{-1}$. If one assumes $L=2$, then the corresponding values of $s(\ln x_{1,min})$ are 0.073 and 0.080, respectively. At higher temperatures accuracy is lower but even for $b=200\text{ cm}^3\cdot\text{mol}^{-1}$, $L=2$ at $T=500$ K value of $s(\ln x)$ does not exceed 0.10, which corresponds to 10% of the calculated hydrocarbon mole fraction. For evaluations presented here it is assumed that data are in good agreement with the reference data when the difference between experimental and reference data does not exceed three times the standard error. Taking upper limit of the relative standard error equal to 10% we specify the experimental solubilities differing from the reference data more than 30% as "doubtful." If at least two experimental points from different sources but measured at similar temperatures, agree with the reference data within the 30% limit, these points are "recommended." If the experimental points for given systems are measured by one laboratory, they are "tentative," even if they agree with the reference data.

Derivation of Reference Data for Solubility of Water in Hydrocarbons

Reference data for the solubility of water in a hydrocarbon were calculated by a method developed by Góral.[6] This method (EoSC) is based on the RK EoS with an added term, which accounts for hydrogen bonding. Application of the EoSC for water systems is described in Maczynski *et al.*[4] and Góral.[5] The input information for this LLE correlation is the solubility of hydrocarbon in water, calculated with Eq. (3), where $\ln x_{1,min}$ and $(\Delta_{sln}C_p/R)$ are calculated with Eqs. (5) and (7). The output is water solubility (x_2) in the hydrocarbon as a function of temperature. The experimental solubility of water was used only at the beginning to fix parameters in the model of the association.

The calculated results were compared with experimental data in Maczynski *et al.*[4] and Góral.[5] The conclusion is that the calculated solubilities of water in alkanes can be used as reference data up to about 60 K below three phase temperature.

For alkenes three systems measured by the same laboratory over a wide temperature range have been reported. The reference data agree well with these experimental data up to about 60 K below the three phase critical temperature but more data are necessary to draw a definite conclusion. Unfortunately, for other unsaturated hydrocarbons solubility of water is reported only up to about 330 K. In view of the accuracy of the experimental data, the agreement between the reference and experimental data is very good but outside of this range the reference data should be treated with care.

Standard error of the water solubility measurements was estimated with the equation:

$$s(\ln x_{2,exp}) = [\Sigma(\ln x_{2,exp} - \ln x_{2,EoSC})_k/(m-n)]^{0.5}, \tag{9}$$

where $\ln x_{2,exp}$ is logarithm of the experimental mole fraction of water in a hydrocarbon and $\ln x_{2,EoSC}$ is the corresponding value calculated with EoSC using n parameters in the model of association. The summation goes through m experimental points. For alkanes $m=148$, $n=4$ and $s(\ln x_{2,exper})=0.27$. Using these values, the average standard error of the reference data was estimated with the equation:

$$\overline{s(\ln x_{2,EoSC})} = s(\ln x_{2,exp})(n/m)^{0.5} \tag{10}$$

Eq. (10) yielded: $\overline{s(\ln x_{2,EoSC})}=0.044$. A somewhat larger value was obtained for unsaturated hydrocarbons. This good agreement is partially caused by the fact that the calculated water solubility is relatively insensitive to errors in the hydrocarbon solubility used as the input data. Nevertheless, to be conservative the same criteria as those listed in previous section were adopted for the recommended, tentative, and doubtful data.

For convenience of the user the solubility data predicted with EoSC were approximated with Eq. (11) proposed by Economou *et al.*[7]

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1-T_r)^{1/3} + d_4(1-T_r). \tag{11}$$

Originally $T_r = T/T_{3c}$, where T_{3c} is three phase critical temperature. In most cases, T_{3c} is not known, therefore instead of T_{3c} an adjustable temperature T^0 is used in Eq. (11). The range of applicability of Eq. (11) is the same as those listed above for EoSC.

1.3. Acknowledgments

The authors are grateful to their many colleagues who have contributed to the IUPAC Solubility Data Project, especially to the compilation and evaluation of hydrocarbon-water systems. In particular, we thank Geraldine Dalton and her colleagues at the U.S. National Institute of Standards and Technology for conversion of the text of Solubility Data Series Volumes 37 and 38 to electronic form.

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1.4. References for the Preface

[1] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 37, *Hydrocarbons with Water and Seawater*, Part I: Hydrocarbons C_5 to C_7 (Pergamon Press, New York, 1989).
[2] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 38, *Hydrocarbons with Water and Seawater*, Part II: Hydrocarbons C_8 to C_{36} (Pergamon Press, New York, 1989).
[3] A. Maczynski, M. Goral, B. Wisniewska-Goclowska, A. Skrzecz, and D. Shaw, Monatshefte für Chemie **134**, 633 (2003).
[4] A. Maczynski, B. Wisniewska-Goclowska, and M. Góral, J. Phys. Chem. Ref. Data **33**, 549 (2004).
[5] M. Góral, B. Wisniewska-Goclowska, and A. Maczynski, J. Phys. Chem. Ref. Data **33**, 579 (2004).
[6] M. Góral, Fluid Phase Equilibria **27**, 118 (1996).
[7] I. G. Economou and C. Tsonopoulos, Chem. Eng. Sci. **52**, 511 (1997).

2. Introduction to the Solubility Data Series: Solubility of Liquids in Liquids

2.1. The Nature of the Project

The Solubility Data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids, and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from different sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

This series is concerned primarily with liquid-liquid systems, but a limited number or related solid-liquid, fluid-fluid and multicomponent (organic water salt) systems are included where it is considered logical and appropriate. Solubilities at elevated and low temperatures and at elevated pressures have also been included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps and upper and lower critical solution temperatures are included where appropriate and when available.

2.2. Compilations, Evaluations, and Quantities and Units Used in Compilation and Evaluation of Solubility Data

Formats for the compilations and critical evaluations have been standardized for all volumes, and complete details for these formats can be found in previous *Solubility Data Series* volumes, for example, Sazonov and Shaw.[1]

Solubilities of liquids in liquids and solids in liquids have been the subject of research for a long time, and have been expressed in a great many ways. The nomenclature, use of-symbols and units in the *IUPAC-NIST Solubility Data Series* follow, where possible, Mills *et al.*,[2] again reviewed in detail in Sazonov and Shaw.[1] A few quantities follow the ISO standards[3] or the German standard;[4] see a review by Cvitaš[5] for details.

A note on nomenclature. The nomenclature of the IUPAC *Green Book*[2] calls the solute component B and the solvent component A. In compilations and evaluations, the first-named component (component 1) is the solute, and the second (component 2 for a two-component system) is the solvent. The reader should bear these distinctions in nomenclature in mind when comparing equations given here with those in the *Green Book*.

2.3. References for the Introduction to the Solubility of Liquids in Liquids

[1] V. P. Sazonov and D. G. Shaw, editors, *Acetonitrile Binary Systems*, IUPAC-NIST Solubility Data Series, Vol. 79, J. Phys. Chem. Ref. Data, **31**(4), 989 (2002).
[2] I. Mills *et al.*, eds. *Quantities, Units and Symbols in Physical Chemistry* (the *Green Book*) (Blackwell Scientific Publications, Oxford, UK, 1993).
[3] ISO Standards Handbook, *Quantities and Units* (International Standards Organization, Geneva, 1993).
[4] German Standard, DIN 1310, *Zusammungsetzung von Mischphasen* (Beuth Verlag, Berlin, 1984).
[5] T. Cvitaš, Chem. International **17**(4), 123 (1995).

3. C_5 Hydrocarbons with Water

3.1. 1,3-Cyclopentadiene

Components:	**Original Measurements:**
(1) 1,3 Cyclopentadiene; C_5H_6; [542-92-7] (2) Water; H_2O; [7732-18-5]	A. Streitweiser and L. L. Nebenzahl, J. Am. Chem. Soc. **98**, 2188 (1976).
Variables:	**Prepared By:**
Room Temperature	M. C. Haulait-Pirson and G. T. Hefter

Experimental Values

The solubility of cyclopentadiene in water at room temperature was reported to be 0.0103 mol·(1)/L sln. [According to a footnote in the paper the experimental data were apparently obtained by J. Cambray (presumably *unpublished observation*) but experimental details are given in the paper.]

Assuming a solution density of 1.00 g/mL the corresponding mass percent and mole fraction (x_1) solubilities, calculated by the compilers, are 0.068 g(1)/100 g sln and $1.8\cdot10^{-4}$ respectively.

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
Water was saturated by shaking with excess (1) and then centrifuged. The saturated solution so obtained was then diluted and analyzed by UV spectrophotometry assuming the absorptivity to be the same as in ethanol.	(1) Aldrich; distilled onto molecular sieves and used within 1h; analyzed by gc. (2) Distilled; purity not specified. **Estimated Error:** Not given.

3.2. Cyclopentene*

Components:	**Evaluator:**
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, May, 2003.

Critical Evaluation of the Solubility of Cyclopentene (1) in Water (2)

The experimental solubility data for cyclopentene (1) in water (2) have been investigated by McAuliffe,[1] Natarajan and Venkatachalam[2] at 298 K, and Pierotti and Liabastre[3] at 298 K and 308 K.

The Evaluators obtained the reference solubility data for cyclopentene (1) in water (2) by the procedures described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{sln}C_p/R)[T_{\min}/T - \ln(T_{\min}/T) - 1],$$

where: $\ln x_{1,\min} = -8.57$; $\Delta_{sln}C_p/R = 28.8$; $T_{\min} = 298$ K.

All the experimental and reference data are listed in the Table 1. The data of McAuliffe,[1] and Natarajan and Venkatachalam[2] at 298 K are in good agreement with each other and with the reference data and are recommended. The data of Pierotti and Liabastre[3] at 298 K and 308 K are in poor agreement with the reference data and are doubtful.

References:

[1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[2]G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng.Data **17**, 328 (1972).

[3]R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

TABLE 1. Solubility of cyclopentene (1) in water (2)

T/K	Experimental values x_1	Reference values: $x_1 \pm 30\%$
298.2	$1.41\cdot10^{-4}$ (McAuliffe[1]), $1.62\cdot10^{-4}$ (Natarajan and Venkatachalam[2])	$1.9\cdot10^{-4}$
298.3	$4.35\cdot10^{-4}$ (Pierotti and Liabastre[3])	$1.9\cdot10^{-4}$
308.4	$4.62\cdot10^{-4}$ (Pierotti and Liabastre[3])	$1.9\cdot10^{-4}$

Components:	Original Measurements:
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of cyclopentene in water at 25 °C was reported to be 535 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0535 g(1)/100 g sln and 1.41×10^{-4}.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250 mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 20 mg(1)/kg (2) (standard deviations of the mean).

Components:	Original Measurements:
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson and G. T. Hefter

Experimental Values

The solubility of cyclopentene in water was reported to be $8.978\cdot10^{-3}$ mol·/L at 25 °C. (It should be noted that although the authors states that the solubility refers to "water"—the context in the paper is ambiguous and the data were probably obtained in 0.001 mol/L HNO_3 solution.)

Assuming a solution density of 1.00 g/mL the corresponding mass percent and mole fraction x_1 solubilities, calculated by the compilers are, respectively, 0.0611 $g(1)$/100 g sln and $1.62\cdot10^{-4}$.

Solubility data are also presented as a function of temperature in various salt solutions.

Auxiliary Information

Method/Apparatus/Procedure:

15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostated glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the (1) content was determined by titration with bromine using standard procedures.

Source and Purity of Materials:

(1) Prepared by dehydration of cyclopentanol and then washed, dried, and fractioned. Purity (not specified) was determined by chromatography.
(2) Not specified.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: not specified.

Components:	**Original Measurements:**
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
Variables:	**Prepared By:**
Temperature: 298.26–308.36 K	M. C. Haulait-Pirson

Experimental Values

Solubility of cyclopentene in water

T/K	$10^3 \cdot x_1$	$g(1)$/100 g sln
298.26	0.4350	0.1645 ± 0.0049
308.36	0.4623	0.1748 ± 0.0044

Auxiliary Information

Method/Apparatus/Procedure:

10 mL of (2) were placed along with 4–10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 h. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 h. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions, and calculation are not given in the paper.

Source and Purity of Materials:

(1) K & K Laboratories, Inc.; 95%–99%; used as received.
(2) Laboratory distilled water.

Estimated Error:

Solubility standard deviations from at least 15 measurements are given above

3.3. 2-Methyl-1,3-butadiene*

Components:	**Evaluator:**
(1) 2-Methyl-1,3-butadiene; C_5H_8; [78-79-5] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, May, 2003.

Critical Evaluation of the Solubility of 2-Methyl-1,3-butadiene (1) in Water (2)

The experimental solubility data for 2-methly-1,3-butadiene (1) in water (2) have been investigated by McAuliffe[1] at 298 K and Pavlova *et al.*[2] at 293–333 K.

Reference solubility data for 2-methly-1,3-butadiene (1) in water (2) were obtained by the Evaluators by the procedures described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{sln}C_p/R)[T_{\min}/T - \ln(T_{\min}/T) - 1],$$

where: $\ln x_{1,\min} = -8.90$; $\Delta_{sln}C_p/R = 32.4$; $T_{\min} = 306$ K.

All the experimental and reference data are listed in Table 2. Since only one experimental data point is available at each temperature, no data can be **recommended**. The data of McAuliffe[1] at 298 K and Pavlova *et al.*[2] at 293 K and 313 K are in good agreement with the reference data and are **tentative**. The data of Pavlova *et al.*[2] at 323 K and 333 K are in poor agreement with the reference data and are **doubtful**.

Critical Evaluation of the Solubility of Water (2) in 2-Methyl-1,3-butadiene (1)

Pavlova *et al.*[2] investigated the experimental solubility data for water (2) in 2-methyl-1,3-butadiene (1) at 293–333 K.

The Evaluator obtained the reference solubility data for (2) in (1) by the method described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r),$$

where $d_1 = -1.358$; $d_2 = -2.481$; $d_3 = 0.394$; $d_4 = -9.823$; $T_r = T/476.1$.

The experimental and reference solubility data for (2) in (1) are listed in Table 3. The data of Pavlova *et al.*[2] at 313 K and 333 K are in good agreement with the reference data and are tentative. The data of Pavlova *et al.*[2] at 293 K are in poor agreement with the reference data and are doubtful.

References:

[1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[2]S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Prom-st Sint. Kauch. **3**, 18 (1966).

TABLE 2. Solubility of 2-methyl-1,3-butadiene (1) in water (2)

T/K	Experimental values x_1	Reference values: $x_1 \pm 30\%$
293.2	$1.44 \cdot 10^{-4}$ (Pavlova *et al.*[2])	$1.4 \cdot 10^{-4}$
298.2	$1.70 \cdot 10^{-4}$ (McAuliffe[1])	$1.4 \cdot 10^{-4}$
313.2	$1.76 \cdot 10^{-4}$ (Pavlova *et al.*[2])	$1.4 \cdot 10^{-4}$
323.2	$2.01 \cdot 10^{-4}$ (Pavlova *et al.*[2])	$1.4 \cdot 10^{-4}$
333.2	$2.29 \cdot 10^{-4}$ (Pavlova *et al.*[2])	$1.5 \cdot 10^{-4}$

TABLE 3. Solubility of water (2) in 2-methyl-1,3-butadiene (1)

T/K	Experimental values x_2	Reference values: $x_2 \pm 30\%$
293.2	$2.26 \cdot 10^{-3}$ (Pavlova *et al.*[2])	$1.7 \cdot 10^{-3}$
313.2	$3.58 \cdot 10^{-3}$ (Pavlova *et al.*[2])	$3.2 \cdot 10^{-3}$
333.2	$5.53 \cdot 10^{-3}$ (Pavlova *et al.*[2])	$6.1 \cdot 10^{-3}$

Components:
(1) 2-Methyl-1,3-butadiene; C_5H_8; [78-79-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of 2-methyl-1,3-butadiene in water at 25 °C was reported to be 642 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0642 g (1)/100 g sln and 1.70×10^{-4}.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 10 mg (1)/kg(2) (standard deviation of mean).

Components:
(1) 2-Methyl-1,3-butadiene; C_5H_8; [78-79-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Prom-st Sint. Kauch. **3**, 18 (1966).

Variables:
Temperature: 20 °C–60 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of 2-methyl-1,3-butadine in water

t/°C	$10^4 \cdot x_1$	g(1)/100 g sln (compiler)
20	1.441	0.05448
40	1.758	0.06646
50	2.013	0.07609
60	2.294	0.08671

Solubility of water in 2-methyl-1,3-butadine

t/°C	$10^3 \cdot x_2$	g(2)/100 g sln (compiler)
20	2.26	0.0598
40	3.58	0.0949
60	5.53	0.1468

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

Source and Purity of Materials:
(1) Source not specified; better than 99.7 wt %.
(2) Doubly distilled.

Estimated Error:
Temperature: ±0.1 °C.

3.4. 1,4-Pentadiene

Components:

(1) 1,4-Pentadiene; C_5H_8; [591-93-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Components:

One temperature: 25 °C

Prepared By:

A. Maczynski, Z. Maczynska, and A. Szafranski

Exerimental Values

The solubility of 1,4-pentadiene in water at 25 °C was reported to be 558 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0558 $g(1)$/100 g sln and 1.48×10^{-4}.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 27 mg (1)/kg (2) (standard deviation of mean).

3.5. 1-Pentyne*

Components:

(1) 1-Pentyne; C_5H_8; [627-19-0]
(2) Water; H_2O; [7732-18-5]

Evaluators:

A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, May, 2003.

Critical Evaluation of the Solubility of 1-Pentyne (1) in Water (2)

McAuliffe[1] and Tewari *et al.*[2] have investigated the experimental solubility for 1-pentyne (1) in water (2) at 298 K.

The Evaluators obtained the reference solubility data for 1-pentyne (1) in water (2) by the procedure described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{sln}C_p/R)[T_{\min}/T - \ln(T_{\min}/T) - 1],$$

where: $\ln x_{1,\min} = -7.95$; $\Delta_{sln}C_p/R = 31.2$; $T_{\min} = 306$ K.

All the experimental and reference data are listed in the Table 4. The data of McAuliffe[1] and Tewari *et al.*[2] at 298 K are in good agreement with each other and with the reference data and are recommended.

References

[1] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[2] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 1982).

TABLE 4. Solubility of 1-pentyne (1) in water (2)

T/K	Experimental values x_1	Reference values: $x_1 \pm 30\%$
298.2	$4.15 \cdot 10^{-4}$ (McAuliffe[1]), $2.78 \cdot 10^{-4}$ (Tewari *et al.*[2])	$3.6 \cdot 10^{-4}$

Components:
(1) 1-Pentyne; C_5H_8; [627-19-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of 1-pentyne in water at 25 °C was reported to be 1570 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.1570 $g(1)$/100 g sln and $4.15 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 33 mg (1)/kg (2) (standard deviation of mean).

Components:
(1) 1-Pentyne; C_5H_8; [627-19-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1-pentyne in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$1.54 \cdot 10^{-2}$	0.1053	$2.78 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with an organic liquid by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by glc. The column was thermostated by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:
(1) Source not specified; purity >99 mole% checked by high-temperature glc.
(2) Source not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 1 % (estimated by the authors).

References:
[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

3.6. Cyclopentane*

Components:
(1) Cyclopentane; C_5H_{10}; [287-92-3]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2003.

Critical Evaluation of the Solubility of Cyclopentane (1) in Water (2)

The following authors have investigated the experimental solubility data for cyclopentane (1) in water (2):

Author (s)	T/K	Author (s)	T/K
Groves[2]	298	Pierotti and Liabastre[5]	278–318
Guseva and Parnov[3]	326–472	Price[6]	298–426
McAuliffe[4]	298		

The Evaluators obtained the reference solubility data for cyclopentane (1) in water (2) by the procedures described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{sln}C_p/R)[T_{\min}/T - \ln(T_{\min}/T) - 1],$$

where: $\ln x_{1,\min} = -10.12$; $\Delta_{sln}C_p/R = 30.8$; $T_{\min} = 298$ K.

The experimental data of Groves,[2] McAuliffe,[4] and Price[6] as well as reference data are listed in Table 5. All the data are shown Fig. 4. The data of Groves,[2] McAuliffe,[4] and Price[6] at 298 K are in good agreement with each other and with the reference data and are recommended. The data of Price[6] at 313–426 K are in good agreement with the reference data and are tentative. The data of Guseva and Parnov,[3] and Pierotti and Liabastre[5] are in poor agreement with the reference data and are doubtful.

Critical Evaluation of the Solubility of Water (2) in Cyclopentane (1)

The experimental solubility of water (2) in cyclopentane (1) has been investigated by Englin[1] at 273–313 K.

The reference solubility data for (2) in (1) were obtained by the Evaluators by the method described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r),$$

where $d_1 = -1.397$; $d_2 = -6.191$; $d_3 = -0.339$; $d_4 = -4.792$; $T_r = T/503.1$.

The experimental and reference solubility data for (2) in (1) are listed in Table 6. All the data are in poor agreement with the reference data and are doubtful.

Rejected Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[8] are independent data. The data reported by Gill *et al.*[7] lack sufficient information to justify evaluation. Therefore these data are rejected.

References:

[1] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[2] F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).
[3] A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).
[4] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[5] R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
[6] L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[7] S. J. Gill, N. F. Nichols, and I. Wadso, J. Chem. Thermodyn. **8**, 445 (1976).
[8] T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

TABLE 5. Solubility of cyclopentane (1) in water (2)

T/K	Experimental values x_1	Reference values $x_1 \pm 30\%$
278.3	$8.70 \cdot 10^{-5}$ (Pierotti and Liabastre[5])	$4.6 \cdot 10^{-5}$
288.4	$8.78 \cdot 10^{-5}$ (Pierotti and Liabastre[5])	$4.4 \cdot 10^{-5}$
298.2	$4.22 \cdot 10^{-5}$ (Groves[2]), $4.00 \cdot 10^{-5}$ (McAuliffe[4]), $4.11 \cdot 10^{-5}$ (Price[6])	$4.3 \cdot 10^{-5}$
298.3	$8.78 \cdot 10^{-5}$ (Pierotti and Liabastre[5])	$4.3 \cdot 10^{-5}$
308.4	$9.46 \cdot 10^{-5}$ (Pierotti and Liabastre[5])	$4.4 \cdot 10^{-5}$
313.3	$4.19 \cdot 10^{-5}$ (Price[6])	$4.5 \cdot 10^{-5}$
318.4	$8.77 \cdot 10^{-5}$ (Pierotti and Liabastre[5])	$4.6 \cdot 10^{-5}$
326.2	$1.10 \cdot 10^{-4}$ (Guseva and Parnov[3])	$4.9 \cdot 10^{-5}$
328.9	$4.62 \cdot 10^{-5}$ (Price[6])	$5.0 \cdot 10^{-5}$
372.3	$7.61 \cdot 10^{-5}$ (Price[6])	$8.7 \cdot 10^{-5}$
390.2	$3.87 \cdot 10^{-4}$ (Guseva and Parnov[3])	$1.2 \cdot 10^{-4}$
391.2	$9.56 \cdot 10^{-5}$ (Price[6])	$1.2 \cdot 10^{-4}$
410.5	$1.57 \cdot 10^{-4}$ (Price[6])	$1.8 \cdot 10^{-4}$
426.3	$2.04 \cdot 10^{-4}$ (Price[6])	$2.5 \cdot 10^{-4}$
439.2	$1.12 \cdot 10^{-3}$ (Guseva and Parnov[3])	$3.3 \cdot 10^{-4}$
471.7	$3.30 \cdot 10^{-3}$ (Guseva and Parnov[3])	$7.1 \cdot 10^{-4}$

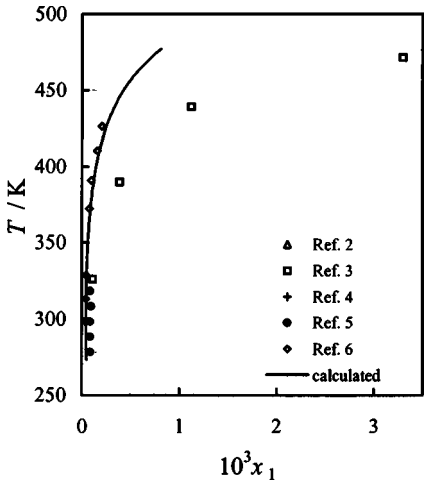

FIG. 4. All the solubility data for cyclopentane (1) in water (2).

TABLE 6. Solubility of water (2) in cyclopentane (1)

T/K	Experimental values x_2	Reference values $x_2 \pm 30\%$
273.2	$1.79 \cdot 10^{-4}$ (Englin *et al.*[1])	$1.1 \cdot 10^{-4}$
283.2	$3.35 \cdot 10^{-4}$ (Englin *et al.*[1])	$1.9 \cdot 10^{-4}$
293.2	$5.53 \cdot 10^{-4}$ (Englin *et al.*[1])	$3.1 \cdot 10^{-4}$
303.2	$9.69 \cdot 10^{-4}$ (Englin *et al.*[1])	$4.8 \cdot 10^{-4}$
313.2	$1.548 \cdot 10^{-3}$ (Englin *et al.*[1])	$7.4 \cdot 10^{-4}$

Components:	**Original Measurements:**
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 0 °C–40 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in cyclopentane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
0	1.79	0.0046
10	3.35	0.0086
20	5.53	0.0142
30	9.69	0.0249
40	15.48	0.0398

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostated flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:
(1) Cyclopentane; C_5H_{10}; [287-92-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of cylcopentane in water

t/°C	mg (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	164±3.6	0.0164	$4.22 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method similar to Polak and Liu[1] was used. Hydrocarbon (1) was injected into 40 mL vials fitted with Teflon-lined septa containing about 20 mL water and placed in a thermostated bath for 2 weeks. The water layer was analyzed chromatographically (3% SP-1500 on Carbopack B at 150 °C, He carrier gas at 30 mL/min., FID detector). The reported result is average of four replicate determinations.

Source and Purity of Materials:
(1) Aldrich, Chemical Co.; purity 97%; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: as above.

References:
[1]J. Polak and B. C. Y. Liu, Can. J. Chem. **51**, 4018 (1973).

Components:
(1) Cyclopentane; C_5H_{10}; [287-92-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).

Variables:
Temperature: 53 °C–198.5 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of cyclopentane in water

t/°C	$10^4 \cdot x_1$ (compiler)	g(1)/100 g(2)	g(1)/100 g sln (compiler)
53	1.10	0.0427	0.0427
117	3.87	0.151	0.151
166	11.12	0.436	0.434
198.5	32.57	1.288	1.271

Auxiliary Information

Method/Apparatus/Procedure:
Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Parnov.[1] No more details were reported in the paper.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

References:
[1]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).

Components:	Original Measurements:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of cyclopentane in water at 25 °C was reported to be 156 mg (1)/kg sln, (0.0156 g/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is $4.0 \cdot 10^{-5}$.

The same value is also reported in McAuliffe.[1,2]

Auxiliary Information

Method/Apparatus/Procedure:

In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; 99+%; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 9 mg (1)/kg sln (standard deviation from mean).

References:

[1]C. McAuliffe, Nature (London) **200**, 1092 (1963).

[2]C. McAuliffe, C. Amer. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:	Original Measurements:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
Variables:	**Prepared By:**
Temperature: 278.26 K–318.36 K	M. C. Haulait-Pirson

Experimental Values

Solubility of cyclopentane in water

T/K	$10^3 \cdot x_1$	$10^4 \cdot x_1$ (converted by compiler)	g(1)/100 g sln
278.26	0.8697	0.8697	0.03386 ± 0.00087
288.36	0.8777	0.8777	0.03417 ± 0.00102
298.26	0.8782	0.8782	0.03419 ± 0.00067
308.36	0.9465	0.9465	0.03685 ± 0.00110
318.36	0.8772	0.8772	0.03415 ± 0.00100

Auxiliary Information

Method/Apparatus/Procedure:

10 mL of (2) were placed along with 4–10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 h. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 h. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculations are given in the paper.

Source and Purity of Materials:

(1) Matheson, Coleman & Bell, 90.8%; used as received.
(2) Laboratory distilled water.

Estimated Error:

Solubility: standard.deviation from at least 15 measurements are given above.

Components:	**Original Measurements:**
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
Temperature: 25 °C–153.1 °C	F. Kapuku

Experimental Values

Solubility of cyclopentane in water at system pressure

t/°C	$10^5 \cdot x_1$ (compiler)	G (1)/100 g sln (compiler)	mg (1)/kg (2)
25.0	4.11	0.0160	160±2.0
40.1	4.19	0.0163	163±3.0
55.7	4.62	0.0180	180±7.0
99.1	7.61	0.0296	296±16.0
118.0	9.56	0.0372	372±15.0
137.3	15.70	0.0611	611±9.0
153.1	20.36	0.0792	792±74.0

Auxiliary Information

Method/Apparatus/Procedure:

Room-temperature solubility was determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2–4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.
Solubility: range of values given above.

3.7. 2-Methyl-2-butene*

Components:	**Evaluator:**
(1) 2-Methyl-2-butene; C_5H_{10}; [513-35-9] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, May, 2003.

Critical Evaluation of the Solubility of 2-Methyl-2-butene (1) in Water (2)

The experimental solubility data for 2-methly-2-butene (1) in water (2) have been investigated by Natarajan and Venkatachalam[2] at 288–298 K and Pavlova *et al.*[3] at 293–333 K.

The Evaluators obtained the reference solubility data for (1) in (2) by the procedures described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{sln}C_p/R)[T_{\min}/T - \ln(T_{\min}/T) - 1],$$

where: $\ln x_{1,\min} = -9.54$; $\Delta_{sln}C_p/R = 33.8$; $T_{\min} = 306$ K.

All the experimental and reference data are listed in Table 7. The data of Natarajan and Venkatachalam,[2] and Pavlova *et al.*[3] at 293 K are in good agreement with each other and with the reference data and are recommended. The data of Pavlova *et al.*[3] at 313 K are in good agreement with the reference data and are tentative. All other data are in poor agreement with the reference data and are doubtful.

Critical Evaluation of the Solubility of Water (2) in 2-Methyl-2-butene (1)

The experimental solubility data for water (2) in 2-methyl-butene (1) have been investigated by Englin *et al.*[2] at 293 K and Pavlova *et al.*[2] at 293–333 K.

The Evaluators obtained the reference solubility data for (2) in (1) by the method described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r),$$

where $d_1 = -1.408$; $d_2 = -2.941$; $d_3 = 0.381$; $d_4 = -9.576$; $T_r = T/477.9$.

The experimental and reference solubility data for (2) in (1) are listed in Table 8. The data of Englin *et al.*[1] and Pavlova *et al.*[3] at 293 K are in good agreement each other and with the reference data and are recommended. The data of Englin *et al.*[1] at 313 K are in good agreement with the reference data and are tentative. All other data are in poor agreement with the reference data and are doubtful.

References

[1]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[2]G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
[3]S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Prom-st Sint. Kauch. **3**, 18 (1966).

TABLE 7. Solubility of 2-methyl-2-butene (1) in water (2)

T/K	Experimental values x_1	Reference values $x_1 \pm 30\%$
288.2	$9.30 \cdot 10^{-5}$ (Natarajan and Venkatachalam[2])	$7.7 \cdot 10^{-5}$
293.2	$8.80 \cdot 10^{-5}$ (Natarajan and Venkatachalam[2]), $5.63 \cdot 10^{-5}$ (Pavlova *et al.*[3])	$7.5 \cdot 10^{-5}$
298.2	$8.30 \cdot 10^{-5}$ (Natarajan and Venkatachalam[2])	$7.3 \cdot 10^{-5}$
313.2	$6.06 \cdot 10^{-5}$ (Pavlova *et al.*[3])	$7.3 \cdot 10^{-5}$
323.2	$6.42 \cdot 10^{-5}$ (Pavlova *et al.*[3])	$7.6 \cdot 10^{-5}$
333.2	$6.87 \cdot 10^{-5}$ (Pavlova *et al.*[3])	$8.1 \cdot 10^{-5}$

TABLE 8. Solubility of water (2) in 2-methyl-2-butene (1)

T/K	Experimental values x_2	Reference values $x_2 \pm 30\%$
293.2	$1.69 \cdot 10^{-3}$ (Englin *et al.*[1]), $1.51 \cdot 10^{-3}$ (Pavlova *et al.*[3])	$1.3 \cdot 10^{-3}$
313.2	$2.29 \cdot 10^{-3}$ (Pavlova *et al.*[3])	$2.5 \cdot 10^{-3}$
333.2	$3.52 \cdot 10^{-3}$ (Pavlova *et al.*[3])	$4.8 \cdot 10^{-3}$

Components:
(1) 2-Methyl-2-butene; C_5H_{10} ; [513-35-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in 2-methyl-2-butene at 20 °C was reported to be 0.0435 $g(2)$/100 g sln.

The corresponding mole fraction, x_2, calculated by the compilers is $1.69 \cdot 10^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostated flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) 2-Methyl-2-butene; C_5H_{10} ; [513-35-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).

Variables:
Temperature: 15 °C–25 °C

Prepared By:
M. C. Haulait-Pirson, G. T. Hefter

Experimental Values

Solubility of 2-methyl-2-butene in 0.001 mol/L HNO_3 solution

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln[b] (compiler)	$10^3 \cdot$ mol(1)/L sln[a]
15	9.3	0.037	5.15 ± 0.21
20	8.8	0.035	4.88 ± 0.16
25	8.3	0.033	4.71 ± 0.20

[a]Uncertainties stated to be "standard deviations from means."
[b]Assuming a solution density of 1.00 g/mL at all temperatures.

Compiler's note:
Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause the olefin solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol/L HCl.

Auxiliary Information

Method/Apparatus/Procedure:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostated glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.

Source and Purity of Materials:
(1) Prepared by dehydration of *t*-amyl alcohol and then washed, dried, and fractionated. Purity (no specification) was determined by chromatography.
(2) Not specified.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: See table above.

Components:	Original Measurements:
(1) 2-Methyl-2-butene; C_5H_{10} ; [513-35-9] (2) Water; H_2O; [7732-18-5]	S. P. Pavlova, A. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Promyshlennost. Sinteticheskogo Kauchuka **3**, 18 (1966).
Variables:	**Prepared By:**
Temperature: 20 °C–60 °C	A. Maczynski

Experimental Values

Solubility of 2-methyl-2-butene in water

t/°C	$10^5 \cdot x_1$	$g(1)$/100 g sln (compiler)
20	5.63	0.0215
40	6.06	0.0236
50	6.42	0.0250
60	6.87	0.0267

Solubility of water in 2-methyl-2-butene

t/°C	$10^3 \cdot x_2$	$g(2)$/100 g sln (compiler)
20	1.51	0.0388
40	2.29	0.0589
60	3.52	0.0906

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

Source and Purity of Materials:

(1) Source not specified; better than 99.7 mass %.
(2) Doubly distilled.

Estimated Error:

Temperature: ±0.1 °C.

3.8. 3-Methyl-1-butene

Components:	Original Measurements:
(1) 3-Methyl-1-butene; C_5H_{10} ; [563-45-1] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of 3-methyl-1-butene in water at 25 °C was reported to be 130 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0130 $g(1)$/100 g sln and $3.34 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 14 mg (1)/kg (2) (standard deviation of mean).

3.9. 1-Pentene

Components:
(1) 1-Pentene; C_5H_{10}; [109-67-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of 1-pentene in water at 25 °C was reported to be 148 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0148 g(1)/100 g sln and $3.80 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatograph in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 7 mg (1)/kg (2) (standard deviation of mean).

3.10. 2-Pentene

Components:
(1) 2-Pentene; C_5H_{10}; [109-68-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of 2-pentene in water at 25 °C was reported to be 203 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0203 g (1)/100 g sln and 5.21×10^{-5}.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatograph in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 8 mg (1)/kg(2) (standard deviation of mean).

3.11. 2,2-Dimethylpropane

Components:
(1) 2,2-Dimethylpropane; C_5H_{12} ; [463-82-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of 2,2-dimethylpropane in water at 25 °C was reported to be 33.2 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00332 g (1)/100 g sln and 8.30×10^{-6}.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatograph in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 10 mg (1)/kg (2) (standard deviation of mean).

3.12. 2-Methylbutane*

Components:
(1) 2-Methylbutane; C_5H_{12} ; [78-78-4]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2003.

Critical Evaluation of the Solubility of 2-Methylbutane (1) in Water (2)

The authors listed below have investigated the experimental solubility data for 2-methylbutane (1) in water (2).

Author (s)	T/K	Author (s)	T/K
McAuliffe[3]	298	Polak and Lu[5]	273 and 298
Pavlova *et al.*[4]	293–333	Price[6]	298

The Evaluators obtained the reference solubility data for 2-methylbutane (1) in water (2) by the procedures described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1=\ln x_{1,\min}+(\Delta_{sln}C_p/R)[T_{\min}/T-\ln(T_{\min}/T)-1],$$

where: $\ln x_{1,\min}=-11.32$; $\Delta_{sln}C_p/R=36.9$; $T_{\min}=306$ K.

All the experimental and reference data are listed in the Table 9. The data of McAuliffe,[3] Polak and Lu,[5] and Price[6] at 298 K are in good agreement with each other and with the reference data and are recommended. The data of Pavlova *et al.*[4] at 293 K and 313 K, Polak and Lu[5] at 273 K are in good agreement with the reference data and are tentative. The data of Pavlova *et al.*[4] at 323 and 333 K are in poor agreement with the reference data and are doubtful.

Critical Evaluation of the Solubility of Water (2) in 2-Methylbutane (1)

The authors listed below investigated the experimental solubility data for water (2) in 2-methylbutane (1).

Author (s)	T/K	Author (s)	T/K
Black *et al.*[1]	279–295	Pavlova *et al.*[4]	293–333
Englin *et al.*[2]	273–293	Polak and Lu[5]	273 and 298

The Evaluators obtained the reference solubility data for (2) in (1) by the method described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r),$$

where $d_1=-1.706$; $d_2=-6.782$; $d_3=-0.047$; $d_4=-5.509$; $T_r=T/458.7$.

The experimental and reference solubility data for (2) in (1) are listed in Table 10. The data of Black *et al.*[1] at 293 K, Englin *et al.*[2] at 283 K and 293 K, and Pavlova *et al.*[4] at 293 K and 313 K are in good agreement with the reference data and are tentative. All other data are in poor agreement with the reference data and are doubtful.

TABLE 9. Solubility of 2-methylbutane (1) in water (2)

T/K	Experimental values x_1	Reference values $x_1\pm30\%$
273.2	$1.81\cdot10^{-5}$ (Polak and Lu[5])	$1.7\cdot10^{-5}$
293.2	$1.17\cdot10^{-5}$ (Pavlova *et al.*[4])	$1.4\cdot10^{-5}$
298.2	$1.19\cdot10^{-5}$ (McAuliffe[3]), $1.24\cdot10^{-5}$ (Polak and Lu[5]), $1.2\cdot10^{-5}$ (Price[6])	$1.3\cdot10^{-5}$
313.2	$1.44\cdot10^{-5}$ (Pavlova *et al.*[4])	$1.3\cdot10^{-5}$
323.2	$1.75\cdot10^{-5}$ (Pavlova *et al.*[4])	$1.4\cdot10^{-5}$
333.2	$1.98\cdot10^{-5}$ (Pavlova *et al.*[4])	$1.5\cdot10^{-5}$

TABLE 10. Solubility of water (2) in 2-methylbutane (1)

T/K	Experimental values x_2	Reference values $x_2 \pm 30\%$
273.2	$1.28 \cdot 10^{-4}$ (Englin *et al.*[2]), $1.12 \cdot 10^{-4}$ (Polak and Lu[5])	$1.9 \cdot 10^{-4}$
279.2	$1.78 \cdot 10^{-4}$ (Black *et al.*[1]), $1.74 \cdot 10^{-4}$ (Black *et al.*[1]), $1.76 \cdot 10^{-4}$ (Black *et al.*[1])	$2.6 \cdot 10^{-4}$
283.2	$2.37 \cdot 10^{-4}$ (Englin *et al.*[2])	$3.2 \cdot 10^{-4}$
288. 5	$2.6 \cdot 10^{-4}$ (Black *et al.*[1])	$4.2 \cdot 10^{-4}$
293.2	$3.76 \cdot 10^{-4}$ (Black *et al.*[1]), $3.61 \cdot 10^{-4}$ (Black *et al.*[1]), $3.77 \cdot 10^{-4}$ (Black *et al.*[1]), $6.4 \cdot 10^{-4}$ (Pavlova *et al.*[4]), $4.49 \cdot 10^{-4}$ (Englin *et al.*[2])	$5.2 \cdot 10^{-4}$
293.7	$4.02 \cdot 10^{-4}$ (Black *et al.*[1])	$5.4 \cdot 10^{-4}$
294.5	$3.8 \cdot 10^{-4}$ (Black *et al.*[1])	$5.6 \cdot 10^{-4}$
295.0	$3.9 \cdot 10^{-4}$ (Black *et al.*[1])	$5.7 \cdot 10^{-4}$
298.2	$3.85 \cdot 10^{-4}$ (Polak and Lu[5])	$6.6 \cdot 10^{-4}$
313.2	$1.03 \cdot 10^{-3}$ (Pavlova *et al.*[4])	$1.3 \cdot 10^{-3}$
333.2	$2.34 \cdot 10^{-3}$ (Pavlova *et al.*[4])	$3.0 \cdot 10^{-3}$

Rejected Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported Krzyzanowska and Szeliga[7] are independent data. Therefore these data are rejected.

References:

[1]C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).

[2]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

[3]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[4]S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Prom-st. Sint. Kauch. **3**, 18 (1966).

[5]J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

[6]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

[7]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).

Variables:
Temperature: 6 °C–21.8 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of water in 2-methylbutane at a total saturation pressure of 1 atm

t/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln	g (2)/100 g sln (compiler)
15.3	2.6	0.0066[a]	0.0066
21.3	3.8	0.0096[a]	0.0096
21.8	3.9	0.0097[a]	0.0097
6.0	1.78	0.00443	0.00443
6.0	1.74	0.00433	0.00433
6.0	1.76	0.00440	0.00440
20.0	3.76	0.00940	0.00940
20.0	3.61	0.00902	0.00902
20.0	3.77	0.00942	0.00942
20.5	4.02	0.01001	0.01001

[a]Determinations made in glass apparatus.

Auxiliary Information

Method/Apparatus/Procedure:
The method described in Joris and Taylor[1] in which tritium oxide acts as a tracer, was used. Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.

Source and Purity of Materials:
(1) Ohio State University under an American Petroleum Institute Project; purity not specified; used as received.
(2) Not specified.

Estimated Error:
Solubility: a few percent (type of error not specified).

References:
[1]G. G. Joris and H. S. Taylor, J. Chem Phys. **16**, 45 (1948).

Components:
(1) 2-Methylbutane; C_5H_{12} ; [78-78-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 0 °C–20 °C

Prepared By:
A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 2-methylbutane

t/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln
0	1.28	0.0032
10	2.37	0.0059
20	4.49	0.0112

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostated flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) 2-Methylbutane; C_5H_{12} ; [78-78-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966)

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 2-methylbutane in water at 25 °C was reported to be 47.8 mg (1)/kg sln, (0.0478 g (1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 1.19×10^{-5}.
The same value is also reported in McAulifffe.[1,2]

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; 99+%; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 1.6 mg (1)/kg sln (standard deviation of mean).

References:
[1]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[2]C. McAuliffe, C. Amer. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:
(1) 2-Methylbutane; C_5H_{12} ; [78-78-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. P. Pavlova, S. Yu. Pavlov, L. A. Serafimov, and L. S. Kofman, Prom-st Sint. Kauch. **3**, 18 (1966).

Variables:
Temperature: 20 °C–60 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of 2-methylbutane in water

t/°C	$10^5 \cdot x_1$	g (1)/100 g sln (compiler)
20	1.17	0.00469
40	1.44	0.00577
50	1.75	0.00701
60	1.98	0.00793

Solubility of water in 2-methylbutane

t/°C	$10^3 \cdot x_2$	g (2)/100 g sln (compiler)
20	0.64	0.0160
40	1.03	0.0257
60	2.34	0.0585

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

Source and Purity of Materials:
(1) Source not specified; better than 99.7 wt %.
(2) Doubly distilled.

Estimated Error:
Temperature: ±0.1 °C.

Components:
(1) 2-Methylbutane; C_5H_{12} ; [78-78-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C. -Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of 2-methylbutane in water

t/°C	$10^5 \cdot x_1$ (compiler)	mg (1)/kg sln
0[a]	1.81	72.4[c]
25[b]	1.24	49.6[c]

Solubility of water in 2-methylbutane

t/°C	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0[a]	1.12	28[d]
25[b]	3.85	96[e]

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C; (b) ±0.01 °C.
Solubility: (c) ±1.7%; (d) ±4.7%; (e) ±3.1% (mean).

Components:	Original Measurements:
(1) 2-Methylbutane; C_5H_{12} ; [78-78-4] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 2-methylbutane (1) in water (2) at 25 °C and at system pressure was reported to be 48 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0048 g (1)/100 g sln and 1.20×10^{-5}.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.
Solubility: 1 mg (1)/kg (2).

3.13. Pentane*

Components:	Evaluators:
(1) Pentane; C_5H_{12} ; [109-66-0] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland January, 2003.

Critical Evaluation of the Solubility of Pentane (1) in Water (2)

The authors listed below investigated the experimental solubility data for pentane (1) in water (2).

Author (s)	T/K	Author (s)	T/K
Barone *et al.*[1]	298	Nelson and De Ligny[9]	288–303
Führer[4]	298	Pierotti and Liabastre[10]	278–308
Jonsson *et al.*[5]	288–308	Polak and Lu[11]	273 and 298
Korenman and Aref'eva[6]	293	Price[12]	298
McAuliffe[7]	298	Rudakov and Lutsyk[13]	298
Namiot and Bender[8]	293–345	Tewari *et al.*[14]	298

The Evaluators obtained the reference solubility data for pentane (1) in water (2) by the procedures described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_1=\ln x_{1,\min}+(\Delta_{sln}C_p/R)[T_{\min}/T-\ln(T_{\min}/T)-1],$$

where: $\ln x_{1,\min}=-11.50$; $\Delta_{sln}C_p/R=37.8$; $T_{\min}=306$ K.

All the experimental and reference data are listed in Table 11 and shown at Fig. 5. The recommended and tentative data are shown in Fig. 6. The data of Jonsson *et al.*,[5] and Nelson and De Ligny[9] at 293 K and 303 K, and Barone *et al.*,[1] Jonsson *et al.*,[5] McAuliffe,[7] Polak and Lu,[11] Price,[12] Tewari *et al.*,[14] Rudakov and Lutsyk,[13] and Tewari *et al.*[14] at 298 K are in good agreement with each other and with the reference data and are recommended. The data of Jonsson *et al.*[5] at 288 K and 308 K, Nelson and De Ligny[9] at 277 K and 283 K, and Polak and Lu[11] at 273 K are in good agreement with the reference data and are tentative. All other data are in poor agreement with the reference data and are doubtful.

Critical Evaluation of the Solubility of Water (2) in Pentane (1)

The experimental solubility data for water (2) in pentane (1) have been investigated by Black *et al.*[2] at 279–298 K, and Polak and Lu[11] at 273 K and 298 K.

The Evaluators obtained the reference solubility data for (2) in (1) by the method described in the Preface (Sec. 1) and expressed by the equation:

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r),$$

where $d_1=-1.591$; $d_2=-6.577$; $d_3=-0.064$; $d_4=-5.526$; $T_r=T/467.5$.

The experimental and reference solubility data for (2) in (1) are listed in Table 12. The data of Black *et al.*[2] at 298 K are in good agreement with the reference data and are tentative. All other data are in poor agreement with the reference data and are doubtful.

High Pressure Solubility of Pentane (1) in Water (2)

Connolly[3] investigated the experimental high pressure solubility of (1) in (2) at constant temperatures 573–625 K and 15 200–70 900 kPa. The data measured by one author only have not been critically evaluated.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[16] are independent data. The data reported by Gill *et al.*,[15] Roof,[17] and Wishnia[19] lack sufficient information to justify evaluation. Therefore these data are rejected. The publication of Scheffer[18] was not accesible to the compilers.

References

[1]G. Barone, V. Crescenzi, B. Pispisa, and P. Quandrifoglio, J. Macromol. Chem. **1**, 761 (1966).
[2]C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
[3]J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).
[4]H. Führer, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).
[5]J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).
[6]I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.05.
[7]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[8]A. Yu. Namiot and S. Ya. Bender, Khim. Tekhnol. Topl. Masel **7**, 52 (1960).
[9]H. D. Nelson and C. L. De Ligny, Recl. Trav. Chim. Pays-Bas Belg. **87**, 528 (1968).
[10]R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
[11]J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[12]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[13]E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).
[14]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

[15]S. J. Gill, N. F. Nichols, and I. Wadso, J. Chem. Thermodyn. **8**, 445 (1976).
[16]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).
[17]J. G. Roof, J. Chem. Eng. Data **15**, 301 (1970).
[18]F. E. C. Scheffer, Proc. Roy. Acad. Amsterdam **17**, 834 (1914).
[19]A. Wishnia, J. Phys. Chem. **67**, 2079 (1963).

TABLE 11. Solubility of pentane (1) in water (2)

T/K	Experimental values x_1	Reference values $x_1 \pm 30\%$
273.2	$1.64 \cdot 10^{-5}$ (Polak and Lu[11])	$1.4 \cdot 10^{-5}$
277.2	$1.02 \cdot 10^{-5}$ (Nelson and De Ligny[9])	$1.3 \cdot 10^{-5}$
278.3	$2.73 \cdot 10^{-5}$ (Pierotti and Liabastre[10])	$1.3 \cdot 10^{-5}$
283.2	$1.07 \cdot 10^{-5}$ (Nelson and De Ligny[9])	$1.2 \cdot 10^{-5}$
288.2	$1.07 \cdot 10^{-5}$ (Jonsson *et al.*[5])	$1.2 \cdot 10^{-5}$
288.4	$2.95 \cdot 10^{-5}$ (Pierotti and Liabastre[10])	$1.2 \cdot 10^{-5}$
289.2	$9.00 \cdot 10^{-5}$ (Fühner[4])	$1.2 \cdot 10^{-5}$
293.2	$1.03 \cdot 10^{-5}$ (Jonsson *et al.*[5]), $1.70 \cdot 10^{-4}$ (Korenman and Aref'eva[6]), $2.70 \cdot 10^{-5}$ (Namiot and Bender[8]), $9.80 \cdot 10^{-6}$ (Nelson and De Ligny[9]), $1.01 \cdot 10^{-5}$ (Nelson and De Ligny[9])	$1.1 \cdot 10^{-5}$
298.2	$1.24 \cdot 10^{-5}$ (Barone *et al.*[1]), $1.01 \cdot 10^{-5}$ (Jonsson *et al.*[5]), $9.60 \cdot 10^{-6}$(McAuliffe[7]), $1.19 \cdot 10^{-5}$ (Polak and Lu[11]), $9.90 \cdot 10^{-6}$ (Price[12]), $1.00 \cdot 10^{-5}$ (Rudakov and Lutsyk[13]), $1.02 \cdot 10^{-5}$ (Tewari *et al.*[14])	$1.1 \cdot 10^{-5}$
298.3	$2.82 \cdot 10^{-5}$ (Pierotti and Liabastre[10])	$1.1 \cdot 10^{-5}$
303.2	$1.01 \cdot 10^{-5}$ (Jonsson *et al.*[5]), $1.01 \cdot 10^{-5}$ (Nelson and De Ligny[9])	$1.1 \cdot 10^{-5}$
308.2	$1.01 \cdot 10^{-5}$ (Jonsson *et al.*[5])	$1.1 \cdot 10^{-5}$
308.4	$2.72 \cdot 10^{-5}$ (Pierotti and Liabastre[10])	$1.1 \cdot 10^{-5}$
311.0	$3.90 \cdot 10^{-5}$ (Namiot and Bender[8])	$1.1 \cdot 10^{-5}$
313.3	$9.90 \cdot 10^{-6}$ (Price[12])	$1.1 \cdot 10^{-5}$
328.9	$1.04 \cdot 10^{-5}$ (Price[12])	$1.2 \cdot 10^{-5}$
344.6	$6.40 \cdot 10^{-5}$ (Namiot and Bender[8])	$1.4 \cdot 10^{-5}$
372.3	$1.73 \cdot 10^{-5}$ (Price[12])	$2.2 \cdot 10^{-5}$
394.5	$2.74 \cdot 10^{-5}$ (Price[12])	$3.4 \cdot 10^{-5}$
410.5	$5.01 \cdot 10^{-5}$ (Price[12])	$4.8 \cdot 10^{-5}$
422.7	$7.43 \cdot 10^{-5}$ (Price[12])	$6.5 \cdot 10^{-5}$

TABLE 12. Solubility of water (2) in pentane (1)

T/K	Experimental values x_2	Reference values $x_2 \pm 30\%$
273.2	$1.04 \cdot 10^{-4}$ (Polak and Lu[11])	$1.8 \cdot 10^{-4}$
278.7	$1.44 \cdot 10^{-4}$ (Black *et al.*[2])	$2.4 \cdot 10^{-4}$
288.2	$2.45 \cdot 10^{-4}$ (Black *et al.*[2])	$3.9 \cdot 10^{-4}$
298.0	$4.77 \cdot 10^{-4}$ (Black *et al.*[2]), 4.81 (Black *et al.*[2])	$6.2 \cdot 10^{-4}$
298.2	$4.04 \cdot 10^{-4}$ (Polak and Lu[11])	$6.3 \cdot 10^{-4}$

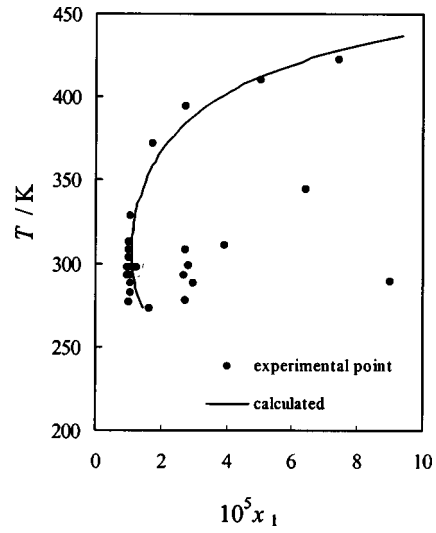

FIG. 5. All the solubility data for pentane (1) in water (2).

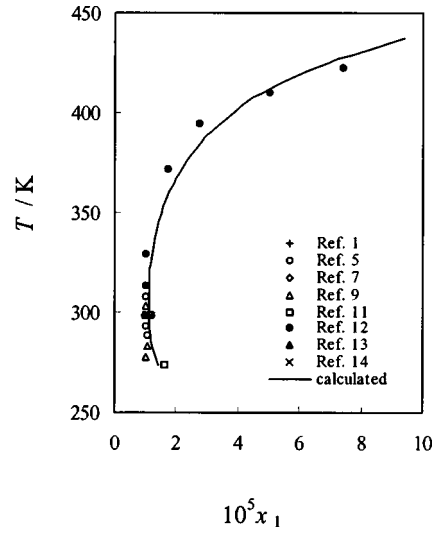

FIG. 6. Recommended and tentative solubility data for pentane (1) in water (2).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. Barone, V. Crescenzi, B. Pispisa, and P. Quandrifoglio, J. Macromol. Chem. **1**, 761 (1966).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The authors report a value of 0.00103 mol (1)/L (2) for the solubility of pentane in water at 25 °C. This value is the experimental one multiplied by 760/P, where P is the partial pressure at (1) over (2). $P = 508$ mm Hg.

The solubility of system pressure calculated by the compiler is 6.88×10^{-4} mol(1)/L(2) and the corresponding mass percent and mole fraction, x_1, are 0.00497g (1)/100 g sln and 1.24×10^{-5} (with the assumption of a solution density of 1 g/mL).

Auxiliary Information

Method/Apparatus/Procedure:
The saturation was carried out by bubbling the vaporized (1) into the solution and letting an excess of the condensed (1) stand in contact with the aqueous phase for more than 12 h at 25 °C under gentle shaking. 0.20 mL samples of (2) saturated with (1) were taken with a calibrated syringe and injected into the chromatographic column packed with 15% of poly(propylene glycol) on chromosorb. A gas chromatography unit having a tungsten wire katharometer as detector was employed. More details are given in the paper.

Source and Purity of Materials:
(1) RP product, C. Erba, Milan; chromatographically pure.
(2) Not specified.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±4% (type of error not specified).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).

Variables:
Temperature: 5.5 °C–24.8 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of water in pentane at a total saturation pressure of 1 atm

T/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g(1)	g (2)/100 g sln (compiler)
5.5	1.44	0.0036	0.0036
15.0	2.45	0.0061	0.0061
24.8	4.77	0.0119	0.0119
24.8	4.81	0.0120	0.0120

Auxiliary Information

Method/Apparatus/Procedure:
The method, described in Joris and Taylor[1] in which tritium oxide acts as a tracer, was used. Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.

Source and Purity of Materials:
(1) Ohio State University under an American Petroleum Institute Project; purity not specified; used as received.
(2) Not specified.

Estimated Error:
Solubility: a few percent (type of error not specified).

References:
[1]G. G. Joris and H. S. Taylor, J. Chem Phys. **16**, 45 (1948).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).

Variables:
Temperature: 300 °C–325 °C
Pressure: 150 atm–700 atm

Prepared By:
M. C. Haulait-Pirson

Experimental Values
Solubility of pentane in water

t/°C	x_1 (compiler)	g (1)/100 g sln	P/atm	P/MPa (compiler)
300	0.0033	1.3	150	15.2
300	0.0043	1.7	185	18.7
300	0.0043	1.7	350	35.4
300	0.0040	1.6	600	60.7
300	0.0038	1.5	700	70.9
330	0.0053	2.1	170	17.2
330	0.0084	3.3	195	19.7
330	0.0103	4.0	220	22.2
330	0.0119	4.6	260	26.3
330	0.0127	4.9	350	35.4
330	0.0122	4.7	485	49.1
330	0.0103	4.0	670	67.8
340	0.0135	5.2	230	23.3
340	0.0160	6.1	250	25.3
340	0.0182	6.9	275	27.8
340	0.0201	7.6	330	33.4
340	0.0201	7.6	350	35.4
340	0.0182	6.9	470	47.6
340	0.0149	5.7	620	62.8
350	0.0207	7.8	240	24.31
350	0.0241	9.0	225	25.83
350	0.0279	10.3	265	26.84
350	0.0332	12.1	280	28.36
350	0.0387	13.9	300	30.39
350	0.0438	15.5	325	32.92
350	0.0438	15.5	350	35.46
350	0.0387	13.9	395	40.01
350	0.0329	12.0	445	45.08
350	0.0279	10.3	510	51.66
350	0.0241	9.0	590	59.77
352	0.0442	15.8	280	28.36
352	0.0533	18.4	280	28.36
352	0.0622	21.0	280	28.36
352	0.0705	23.3	280	28.36
352	0.1463	40.7	400	40.52
352	0.1362	38.7	390	39.51
352	0.1255	36.5	385	39.00
352	0.1140	34.0	380	38.49
352	0.1026	31.4	375	37.99
352	0.0905	28.5	375	37.99
352	0.0784	25.4	375	37.99
352	0.0705	23.3	375	37.99
352	0.0622	21.0	380	38.49
352	0.0533	18.4	390	39.51
352	0.0444	15.7	420	42.55

Comments and Additional Data:
Upper critical solution temperature: 351 °C at $P = 340$ atm.
The uncertainty in the CST is about 2 °C and that of the corresponding pressure about 10 atm.

Auxiliary Information

Method/Apparatus/Procedure:
The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.

Source and Purity of Materials:
(1) Phillips reagent grade; better than 99.8% used as received.
(2) Distilled and deaerated.

Estimated Error:
Temperature: ±0.02 °C.
Pressure: ±2 atm (accuracy).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Führner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).

Variables:
One temperature: 16 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of pentane in water at 16 °C was reported to be 0.060 ml (1)/100 mL sln or 0.036 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler is 9.0×10^{-5}.

Auxiliary Information

Method/Apparatus/Procedure:
In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100 or 1000 mL of (2) until a completely clear solution was obtained at the experimental temperature.

Source and Purity of Materials:
(1) Source not specified; commercial grade; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Pentane; C_5H_{12} ; [109-66-0](2) Water; H_2O; [7732-18-5]

Original Measurements:
J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).

Variables:
Temperature: 15 °C–35 °C

Prepared By:
G. T. Hefter

Experimental Values

Solubility of pentane in water[a]

T/°C	$10^5\cdot x_1$ (compiler)	$10^3\cdot g$(1)/100 g sln (compiler)	mg (1)/kg sln
15	1.07	4.29	42.9
20	1.03	4.14	41.4
25	1.01	4.06	40.6
30	1.01	4.03	40.3
35	1.01	4.06	40.6

[a]Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinitive solution were valid at the saturation pressure of (1).

Auxiliary Information

Method/Apparatus/Procedure:
Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was absorbed in a porous polymer trap and the entrapped (1) analyzed by gas chromatography. The method and apparatus are described in detail in Vejrosta *et al.*[1]

Source and Purity of Materials:
(1) Fluka, >99.8%, used as received.
(2) Not specified.

Estimated Error:
Not specified.

References:
[1]J. Vejrosta, J. Novak, and J. A. Jonsson, Fluid Phase Equilib. **8**, 25 (1982).

Components:	Original Measurements:
(1) Pentane; C_5H_{12} ; [109-66-0] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.05.
Variables:	**Prepared By:**
One temperature: 20 °C	A. Maczynski

Experimental Values

The solubility of pentane in water at 20 °C was reported to be 0.7 g(1)/L(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.07 g(1)/100 g sln and 1.7×10^{-4}.

The assumption that 1 L sln = 1 kg sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

About 100–500 mL (2) was placed in a glass cylinder and 10–50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5–1.5 min.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Pentane; C_5H_{12} ; [109-66-0] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of pentane in water at 25 °C was reported to be 38.5 mg (1)/kg sln, (0.0385g/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 9.6×10^{-6}. The same value is also reported in McAuliffe.[1,2]

Auxiliary Information

Method/Apparatus/Procedure:

In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; 99+ % purity; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 2 mg (1)/kg sln (standard deviation of mean).

References:

[1]C. McAuliffe, Nature (London) **200**, 1092 (1963).

[2]C. McAuliffe, C. Amer. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Yu. Namiot and S. Ya. Bender, Khim. Tekhnol. Topl. Masel **7**, 52 (1960).

Variables:
Temperature: 20 °C–71.4 °C

Prepared By:
A. Maczynski

Experimental Values
Solubility of pentane in water at 32 atm.

T/°C	$10^5 \cdot x_1$	g (1)/100 g sln
20	2.7	0.011
37.8	3.9	0.015
71.4	6.4	0.026

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined from gas-liquid equilibrium measurements in the ternary system pentane-water-methane at 32 atm. In an apparatus described in Rogov *et al.*[1] No more details were reported in the paper

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

References:
[1]B. A. Rogov, A. Yu. Namiot, and M. M. Bondareva, Tr. Vses. Neftegazov. Nach. Issled. Inst. **15**, 196 (1958).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. D. Nelson and C. L. De Ligny, Recl. Trav. Chim. Pays-Bas Belg. **87**, 528 (1968).

Variables:
Temperature: 4 °C–30 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values
Solubility of pentane in water

T/°C	$10^5 \cdot x_1$	mg (1)/kg sln (compiler)
4.0	1.02 ± 0.20	40.9
10.0	1.07 ± 0.15	42.9
20.0	0.98 ± 0.19	39.3
25.0	1.01 ± 0.12	40.5
30.0	1.01 ± 0.17	40.5

Auxiliary Information

Method/Apparatus/Procedure:
The saturation vessel is drawn in the original paper. (2) was saturated with (1) via the vapor phase: a few drops of (1) were put on the bottom of a tight-fitting flask containing a small flask filled with water. Complete saturation was reached by shaking overnight in an upright position. Samples were taken from the aqueous solution with a microsyringe through the septum and injected into the gas chromatograph equipped with a flame ionization detector. The gas chromatographic conditions are described in the paper.

Source and Purity of Materials:
(1) Phillips pure grade.
(2) Tap water was refluxed for 8 h in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more.

Estimated Error:
Solubility: error given above (90% probability interval).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

Variables:
Temperature: 278.26 K–308.36 K

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of pentane in water

T/K	$10^3 \cdot x_1$	g (1)/100 g sln (corrected by compiler)	g (1)/100 g sln
278.26	0.02732	0.01094	0.001094±0.000037
288.36	0.02946	0.01180	0.001180±0.000034
298.26	0.02816	0.01128	0.001128±0.000045
308.36	0.02719	0.01089	0.001089±0.000051

Auxiliary Information

Method/Apparatus/Procedure:
10 mL of (2) were placed along with 4–10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 h. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 h. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified grade; used as received.
(2) Laboratory distilled water.

Estimated Error:
Solubility: standard deviations from at least 15 measurements are given above.

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of water in pentane

t/°C	$10^5 \cdot x_1$ (compiler)	mg (1)/kg sln
0[a]	1.64	65.7[c]
25[b]	1.19	47.6[c]

Solubilityofwaterinpentane

t/°C	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0[a]	1.04	26[d]
25[b]	4.04	101[e]

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C; (b) ±0.01 °C.
Solubility: (c) ±1.7%; (d) ±4.7%; (e) ±3.1% (mean).

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:
Temperature: 25 °C–149.5 °C

Prepared By:
F. Kapuku

Experimental Values

Solubility of pentane in water at system pressure

T/°C	$10^5 \cdot x_1$ (compiler)	g (1)/100 g sln (compiler)	mg (1)/kg (2)
25.0	0.99	0.00395	39.5±0.6
40.1	0.99	0.00398	39.8±0.9
55.7	1.04	0.00418	41.8±1.3
99.1	1.73	0.00694	69.4±1.1
121.3	2.74	0.0110	110.0±10.0
137.3	5.01	0.0201	201.0±5.0
149.5	7.43	0.0298	298.0±14.0

Auxiliary Information

Method/Apparatus/Procedure:
Room-temperature solubility was determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2–4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: range of values given above.

Components:
(1) Pentane; C_5H_{12} ; [109-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The authors reported the partition coefficient α of pentane between the gas and aqueous phase. $\alpha = 49 \pm 1$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25 °C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of P (where P is the vapor pressure in mm of Hg) is taken from Hine and Mooker.[1] $P = 512.5$ mm of Hg and $\log C_g = \log P - 4.269 = -1.56$ expressed in moles per liter. Therefore $C_s = 5.63 \times 10^{-4}$ moles/L.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is $0.0040g$ (1)/100 g sln and the corresponding mole fraction, x_1, is 1.0×10^{-5}.

Auxiliary Information

Method/Apparatus/Procedure:
The equilibrium distribution was attained after shaking for 10 min the thermostated reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Solubility: ±10% (estimated by the compiler).

References:
[1] J. Hine and P. K. Mooker, J. Org. Chem. **4**, 292 (1975).

Components:	**Original Measurements:**
(1) Pentane; C_5H_{12} ; [109-66-0] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of pentane in water

t/°C	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	$5.65 \cdot 10^{-4}$	$4.09 \cdot 10^{-3}$	$1.021 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with an organic liquid by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by glc. The column was thermostated by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:

(1) Source not specified; purity>99 mole % checked by high-temperature glc.
(3) Source not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:

[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

4. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables

5. Registry Number Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables

6. Author Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables